Melt Index Modeling with Support Vector Machines, Partial Least Squares, and Artificial Neural Networks

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ABSTRACT: This article presents the application of three black-box modeling methods to two industrial polymerization processes to predict the melt index, which is considered an important quality variable determining product specifications. The modeling methods covered in this study are support vector machines (SVMs; known as state-of-the-art modeling methods), partial least squares (PLS), and artificial neural networks (ANNs); the processes are styrene–acrylonitrile (SAN) and polypropylene (PP) polymerizations currently operated for commercial purposes in Korea. Brief outlines of the modeling procedure are presented for each method, followed by the procedures for training and validating the models. The SVM models yield the best prediction performances for both the SAN and PP polymerization processes. However, the ANN models fail to accurately predict the melt index when sufficient data are not available for model training in the PP polymerization process. The PLS models are not effective either when applied to the SAN polymerization process, for which the melt index has strong nonlinear functionality with the process variables. The good prediction performance that the SVM models show despite the insufficient data or strong process nonlinearity suggests that SVMs can be effectively used as alternative to PLS or ANNs for modeling the melt indices in other polymerization processes as well. J Appl Polym Sci 95: 967–974, 2005

Key words: computer mechanical properties; modeling; melt; plastics

INTRODUCTION

The melt index of thermoplastic polymers such as polyethylene (PE), polypropylene (PP), and polystyrene (PS) is defined as the mass rate of extrusion flow through a specified capillary under prescribed conditions of temperature and pressure.[1] Because the index determines the flow properties as well as other mechanical properties of polymer products, it is considered one of the important quality variables in the manufacturing process. The measurements of the melt index are used to control the process operating conditions to meet a desired quality of the intermediate or final products.[2]

However, the direct measurement of the melt index in the laboratory is not only costly but also time-consuming and so cannot be conducted frequently enough in practice for proper quality control. Sometimes, these problems make the real-time control of the product quality difficult or even impossible and, therefore, yield off-spec products, resulting in enormous economic losses. Hence, many researchers have strived to infer the melt index indirectly with mathematical models that relate the melt index to other readily measurable process variables. Such modeling approaches have gained increasing feasibility and success on the basis of real-time database systems (RTDBs), which have become widely available in the chemical industry with the rapid growth of information technology. Now we are able to model and analyze polymerization processes more cheaply and quickly with the huge amount of measurement data stored in the RTDBs.

The modeling approaches for the prediction of the melt index can be divided into the following two categories: the mechanistic modeling approaches based on physicochemical principles such as material and energy balances and the black-box modeling approaches based on process operational data from which the input/output functionality can be found with supervisory learning methods such as artificial neural networks (ANNs), partial least squares (PLS), or support vector machines (SVMs). Because this arti-

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cle deals with the prediction of the melt index on the basis of process operation data, we focus only on the black-box modeling methods.

Several works have been carried out to predict melt indices with various types of modeling methods. Ohshima et al.[3] provided an extensive review of the estimation models for polymer properties including the melt index, density, and molecular weight, focusing on the online soft-sensing and optimal-grade changeover control problems for a PE polymerization process. McAuley and MacGregor[4] presented theoretically based models for the online estimation of the melt index and the density in a fluidized-bed ethylene copolymerization reactor. They developed a recursive technique for updating model parameters for the online use of their models and reported successful predictions of the melt index and the density.

In this article, we aim to compare the performances of three black-box modeling methods (SVMs, PLS, and ANNs) for the prediction of the melt indices in two polymerization processes [styrene–acrylonitrile (SAN) and PP]. Unlike PLS or ANNs, SVMs have only recently been introduced and reported to yield successful results in various modeling fields.[5–7] To the best of our knowledge, however, the application of SVMs to polymerization processes has not been reported in the open literature so far; this article appears to be the first to report the use of an SVM for modeling polymerization processes and to compare its performance with the other modeling methods. As is clear from the results to be presented later, the SVM models outperformed the other models in predicting the melt indices of the SAN and PP polymerization processes, and this has led us to recommend their use in other polymerization processes as well.

MELT INDEX MODELING

In this study, three black-box modeling methods (SVMs, PLS, and ANNs) have been used to predict the melt index in the polymerization processes. The SVMs and ANNs are capable of constructing both linear and nonlinear models, but the PLS builds only a linear model. Details on these black-box modeling methods for the melt index are presented in the following.

SVMs

SVMs have been known as very powerful modeling algorithms used to solve classification problems since Vapnik et al.[8] proposed this modeling (learning) strategy. Because the formulation of SVMs is based on structural risk minimization rather than empirical risk minimization, which is employed by other conventional black-box modeling algorithms, including ANNs and PLS, the SVMs typically perform better than the conventional algorithms.[9] In addition, an SVM uses a hypothesis space of linear functions in a high dimensional feature space, trained by solving a convex quadratic optimization problem, and so a global solution is always guaranteed in locating its model parameters. SVMs have a few tunable parameters, such as the capacity constant to control the complexity of functions and the type of kernel function used for transforming the original input space into a high dimensional feature space. For these reasons, SVMs have become increasingly popular alternatives to ANNs.

Recently, the concept of SVMs has been extended to the domain of regression problems.[10] Solving a regression problem with SVMs is called support vector regressions (SVRs), and their applications to many regression problems have yielded excellent performances.[5–7] In this study, a brief sketch of the SVR algorithm is provided; a more detailed description can be found in the literature.[11]

In a regression problem with an SVM, given a training data set of n samples, for which $\mathbf{X}$ is equal to $[\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]^T$ (the matrix of the measured process variables) and $\mathbf{y}$ is equal to $[y_1, y_2, \ldots, y_n]^T$ (the vector of the measured melt index), the unknown functionality is approximated with a finite number of parameters as follows:

$$\hat{y} = f(\mathbf{x},\alpha,\alpha^*) = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)\, K(\mathbf{x},\mathbf{x}_i) + b \qquad (1)$$

where $\hat{y}$ denotes the predicted melt index, α and α^* are the Lagrange multipliers, and $K(\mathbf{x},\mathbf{z})$ is the kernel function, which maps the input space $\mathbf{X}$ implicitly to a feature space. The kernel can be chosen from various types of kernel functions, such as a linear kernel [$K(\mathbf{x},\mathbf{z}) = \mathbf{xz}$], a polynomial kernel [$K(\mathbf{x},\mathbf{z}) = (\mathbf{x}^T\mathbf{z})^d$], or a radial bias function (RBF) kernel [$K(\mathbf{x},\mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|^2/(2\sigma^2)$ where σ is the width of Gaussian]. In this study, the RBF kernel is adopted to model the melt index because it is frequently used for various regression problems for its high resolution power.[5–7] α and α^* are obtained by the solution of the following constrained quadratic programming (QP) problem:

$$\min J(\alpha,\alpha^*) = \varepsilon\sum_{i=1}^{n}(\alpha_i^* + \alpha_i) - \sum_{i=1}^{n} y_i(\alpha_i^* - \alpha_i) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)\, K(\mathbf{x}_i,\mathbf{x}_j) \qquad (2)$$

subject to

$$0 \le \alpha_i^* \le C \quad i = 1, 2, \cdots, n \qquad (3)$$

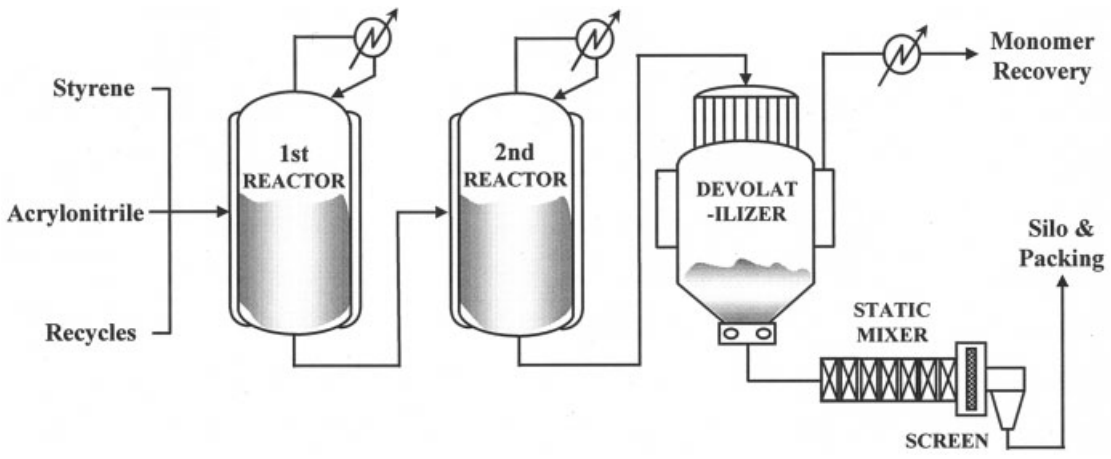


Figure 1 Schematic of SAN polymerization.

$$0 \le \alpha_i \le C \quad i = 1, 2, \cdots, n \tag{4}$$

$$\sum_{i=1}^{n} \alpha_i^* = \sum_{i=1}^{n} \alpha_i \tag{5}$$

where C (the capacity constant) and ε (the size of the ε-insensitive zone of an ε-insensitive loss function[11]) are two tuning parameters used to control the generalization ability of the approximated function [eq. (1)]. They should be adequately determined to obtain good prediction results. In this study, a crossvalidation method[12] has been used, in which the optimal performance is assessed with a separate validation set of the process variables and the melt index. The solutions of the optimization problem described by eqs. (2)–(5) are the vectors $\boldsymbol{\alpha}^*$ and $\boldsymbol{\alpha}$. Most elements of these solution vectors vanish, and the data samples corresponding to non-zero values of α_i^* and α_i are called the support vectors. The bias term b in eq. (1) can be calculated from s training data pertaining to the support vectors obtained as the optimization solutions, and it is a unique constant that minimizes the error over the training data set:

$$\min L(b) = \sum_{j=1}^{s} (y_j - \varepsilon - \sum_{i=1}^{n} (\alpha_i^* - \alpha_i) K(\mathbf{x}, \mathbf{x}_i) - b)^2 \tag{6}$$

To efficiently solve the QP problem described by eqs. (2)–(5), several types of optimization algorithms have been proposed for SVMs. In this study, the sequential minimal optimization algorithm[13] with a decomposition method is employed; it decomposes a large QP problem into a series of smaller QP subproblems.

PLS

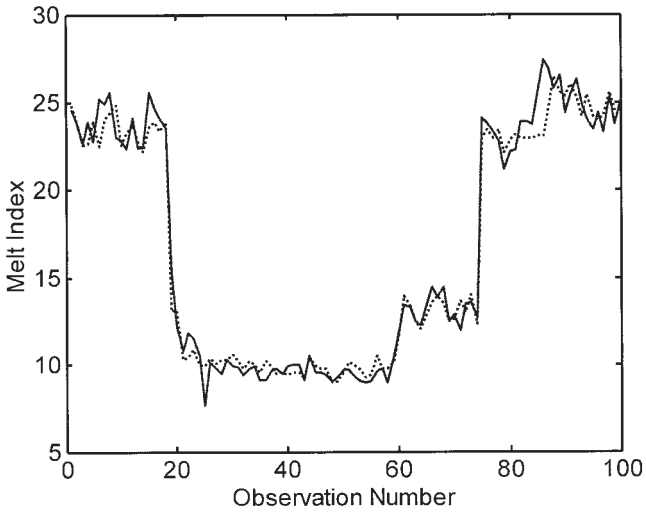
PLS has been widely used as a powerful modeling method for constructing black-box models from laboratory and field measurement data.[14,15] It typically provides more robust and reliable models than ordinary least-squares methods, particularly when the data are noisy and highly correlated with each other.[12,16] The basic concept of PLS regression is to project the high dimensional spaces of the input and output data obtained from a process onto the low dimensional feature (latent) spaces and then to find the best relation between the feature vectors. It is capable of dealing with singular and highly correlated regression problems, which the traditional multiple linear regression methods cannot handle. In addition, it enables the modeling results to be easily interpreted by providing helpful information in the form of scores, loadings, and regression coefficients.

The first step in PLS modeling is to arrange the measurements on v process variables and one quality variable (melt index) at n different sampling times into $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]^T$ and $\mathbf{y} = [y_1, y_2, \ldots, y_n]^T$, respectively. Then, after being scaled and mean-centered, each $\mathbf{X}$ and $\mathbf{y}$ are decomposed as a sum of a series of rank-one matrices or vectors according to the following outer relations:

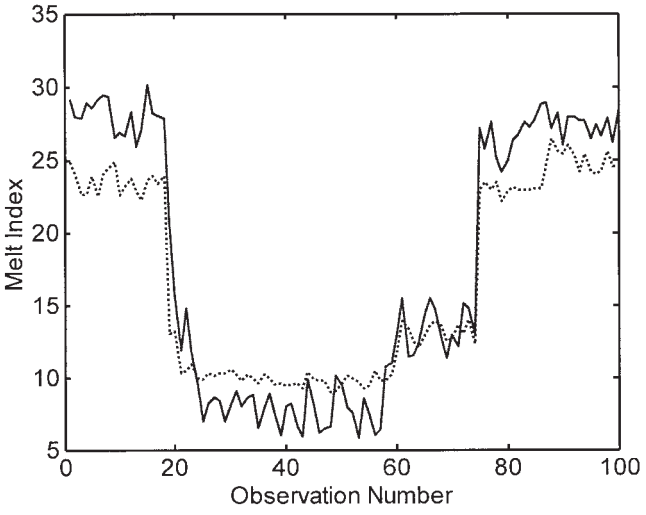
$$\mathbf{X} = \sum_{i=1}^{a} \mathbf{t}_i \mathbf{p}_i^T + \mathbf{E} \tag{7}$$

$$\mathbf{y} = \sum_{i=1}^{a} \mathbf{u}_i q_i^T + \mathbf{f} \tag{8}$$

where $\mathbf{t}_i$ and $\mathbf{u}_i$ represent the input and output score vectors, respectively. They are calculated sequentially from the data for each latent variable i (also called the PLS dimension). The loading vector ($\mathbf{p}_i$) and value of q_i show the influences of $\mathbf{X}$ and $\mathbf{y}$, respectively. All the score and loading vectors are determined so that both the residual matrix ($\mathbf{E}$) and the residual vector ($\mathbf{f}$) are minimized.



(a)



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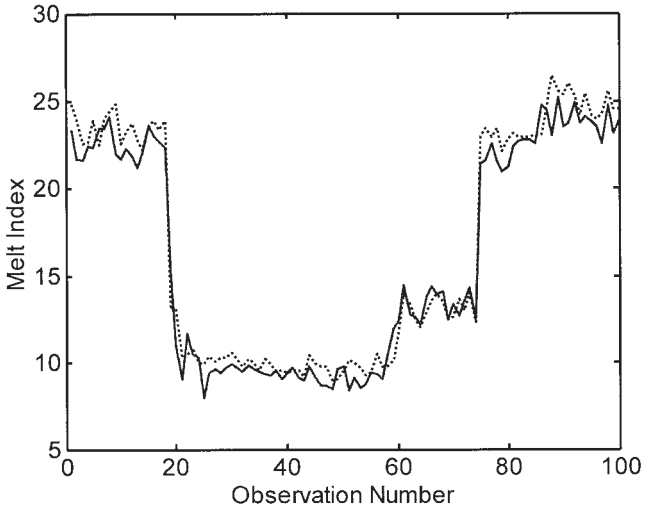


(c)

After the outer relations are obtained, the following linear model is assumed to describe the inner relationship between each $\mathbf{t}_i$ and $\mathbf{u}_i$:

$$\mathbf{u}_i = c_i\mathbf{t}_i + \mathbf{h}_i \quad i = 1, 2, \cdots, a \tag{9}$$

The regression coefficient (c_i) is determined by the minimization of the residual ($\mathbf{h}_i$) for each latent variable i and can be grouped into a diagonal matrix ($\mathbf{C}$), with the off-diagonal elements set equal to zero. Combining eqs. (7)–(9) into one equation, we can obtain the following PLS prediction equation:

$$\hat{\mathbf{y}} = \sum_{i=1}^{a}\mathbf{t}_i c_i q_i^T = \mathbf{TCq}^T = \mathbf{X}(\mathbf{P}^T)^{-1}\mathbf{Cq}^T \tag{10}$$

where $\mathbf{T}$ is equal to $[\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_a]$, $\mathbf{P}$ is equal to $[\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_a]$, $\mathbf{q}$ is equal to $[q_1, q_2, \ldots, q_a]$, and $\hat{\mathbf{y}}$ is equal to $[\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \ldots, \hat{\mathbf{y}}_n]$ (the vector of the predicted values of the melt index). In the previous equation, the total number of latent variables (a) is the only tuning parameter determined by means of crossvalidation[12] and is typically much lower than the number of process variables (v). The regression coefficients ($\mathbf{C}$) are determined from the underlying PLS regression model and can be used to interpret how the process variables ($\mathbf{X}$) are correlated to the quality variable (melt index; $\mathbf{y}$). Typically, the most instructive method for calculating the PLS parameters, including the scores, loadings, and regression coefficients, is known as the nonlinear iterative PLS algorithm,[12] in which the PLS parameters are computed sequentially for each latent variable.

ANNs

ANNs are widely used for modeling the nonlinear behavior of a process because they allow a great deal of flexibility in determining model structures. They typically give good modeling performances when there is a sufficient amount of data.[14,17,18] An ANN consists of a number of interconnected computing processors called neurons or nodes, which are grouped into input, hidden, and output layers. The strengths of the connections among the nodes are called the weights and are adjusted with a suitable learning algorithm to yield good agreement with the observed output. Various types of ANNs have been

Figure 2 Results of melt index modeling (a) with the SVM method, (b) with the PLS method, and (c) with the ANN method for SAN polymerization: (· · ·) measured values and (—) predicted values.

TABLE I
Optimal Tuning Parameters and CPU Time

Modeling method	Tuning parameters and CPU time	SAN polymerization process	PP polymerization process
SVM	C	9.0	1.1
	ε	0.02	0.1
	CPU time	5.4 s	1.5s
PLS	a	10	5
	CPU time	0.2 s	0.2s
ANN	h	5	8
	CPU time	33.8 s	57.9s

The CPU time is the time required to train a model with the optimal tuning parameters and was measured on a Pentium 4.2-GHz machine.

proposed that differ in their structures and learning algorithms.[19]

In this study, the melt index is modeled with a feed-forward network with one hidden layer and the following representation of the function:

$$\hat{y} = f^{(2)}\left(\sum_{i=1}^{h} w_i^{(2)} f_i^{(1)}(\mathbf{x}^T\mathbf{W}_i^{(1)} + b_i^{(1)}) + b^{(2)}\right) \qquad (11)$$

In eq. (11), $\mathbf{x}$ denotes the vector of the process variables of size v, $\hat{y}$ is the melt index to be predicted, and h is the number of nodes in the hidden layer. The transfer function for each hidden node is the sigmoid function represented by $f_i^{(1)}(z) = 1/[1 + \exp(-z)]$, and that for the output node is the pure linear function $f^{(2)}(z) = z$. Because the primary structure of the neural network is constructed by the number of hidden layers and the types of transfer functions being fixed, the only tuning parameter to be sought is h. The model coefficients are the weights ($\mathbf{W} = [\mathbf{w}_1^{(1)}, \mathbf{w}_2^{(1)}, \ldots, \mathbf{w}_h^{(1)}]$ and $[w_1^{(2)}, w_2^{(2)}, \ldots, w_h^{(2)}]$) and the biases ($\mathbf{b} = [b_1^{(1)}, b_2^{(1)}, \ldots, b_h^{(1)}]$ and $b^{(2)}$). Given a training data set of n samples ($\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]^T$ and $\mathbf{y} = [y_1, y_2, \ldots, y_n]^T$), the model coefficients (the weights and the biases) are determined so that the following least-squares objective function is minimized:

$$\min J(\mathbf{W},\mathbf{b}) = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad (12)$$

Generally, the weights and biases in this type of feed-forward network are determined with a backpropagation training algorithm.[20] It has been shown that the network described by eq. (11) can approximate virtually any function of interest to any degree of accuracy, as long as enough hidden units are available.[21] For this kind of multilayer network, however, it is not easy to determine the optimal structure and parameters because the typical minimization process suffers from the existence of many local minima.[17,20]

RESULTS AND DISCUSSION

The black-box modeling methods addressed in the preceding section are applied to the prediction of the melt indices in two industrial polymerization processes: SAN and PP polymerization processes being currently operated for commercial purposes in Korea. In this section, the modeling and prediction results are analyzed, compared, and discussed.

SAN polymerization process

Figure 1 shows the schematic diagram of an SAN polymerization process currently operated for commercial purposes in Korea. The process is capable of producing about 50,000 tons of SAN copolymer per year. First, styrene and acrylonitrile monomers are fed into the first reactor, in which about half of them are polymerized into the SAN copolymer. In the second reactor, the rest of them are further polymerized to achieve over 75% conversion of the styrene. The mixture of the polymer and the monomers is conveyed into the devolatilizer, in which the excess monomers and solvents are recovered. The polymer products are screened through the static mixer to remove impurities and then are stored in silos. The process typically

TABLE II
RSMEs for the Models for Melt Indices

Modeling method	RMSE for the testing data sets: SAN polymerization process	RMSE for the testing data sets: PP polymerization process
SVM	0.97	1.51
PLS	3.15	2.08
ANN	1.09	3.07

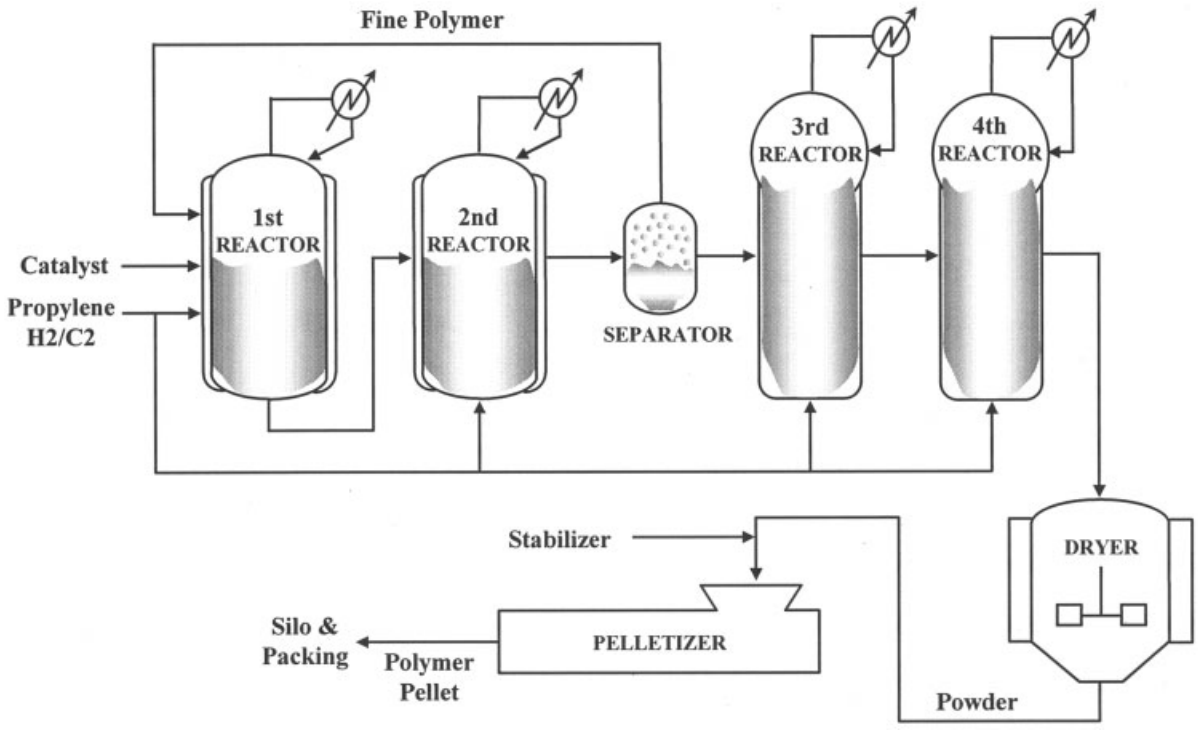


Figure 3 Schematic of PP polymerization.

produces products of about eight different grades, which are altered more than five times per month.

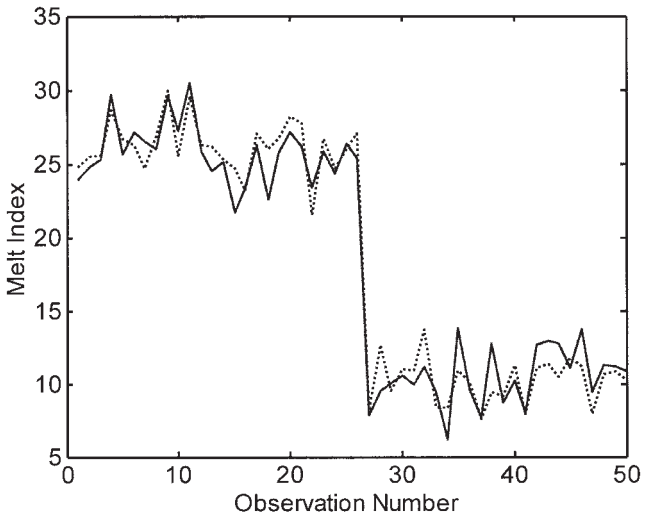
The first step in black-box modeling is to prepare a set of training data measured on the target process of interest. The process variables, such as the temperatures, pressures, and levels, are measured every minute and stored in the RTDB, whereas the quality variables, including the melt index, are measured every 4 h and stored in the laboratory information management system (LIMS). A total of 33 process variables have been selected as the independent variables for modeling the melt index. Because the quality variables are measured much less frequently than the process variables, moving averages of the measurements on the process variables have been taken over a 4-h period before each sampling time for the quality variables. A principal component analysis (PCA)[22] has been employed to eliminate statistical outliers that might result from faulty measurements or abnormal operation to finally obtain a total of 1024 training data (measured for 4096 h). Apart from the training data, a total of 100 testing data (measured for 400 h) have been used to tune and verify each of the SVM, PLS, and ANN models and to compare their performances. Table I summarizes the optimal tuning parameters used for model training to yield the smallest prediction errors for the testing data of the SAN polymerization process.

Figure 2(a–c) compares the measured values with the predicted ones from the SVM, PLS, and ANN models, respectively, for the SAN polymerization process. The prediction performances of the three models can also be assessed from Table II, which lists the root-mean-squared errors (RMSEs) between the measured and predicted values of the melt indices defined as follows:

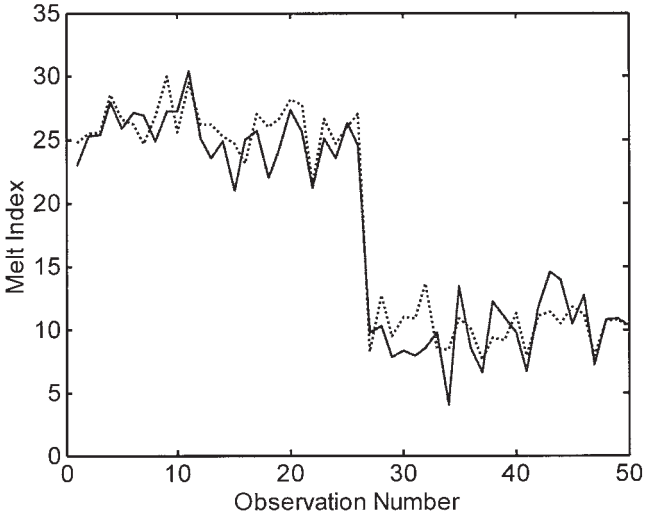
$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{n} (\hat{y}_i - y_i)/n} \tag{13}$$

As shown in the figures and the table, the SVM model yields the best prediction performance: most predicted values track the measured ones very closely throughout the observation period in Figure 2(a), and its RMSE is the smallest of the three models in Table II. In contrast, the PLS model predictions show large deviations from the measured values, especially for the observation numbers up to 18 in Figure 2(b). Furthermore, the RMSE for the PLS model is more than three times larger than that of the SVM model. On the other hand, the ANN model shows a prediction performance comparable to that of the SVM with respect to the tracking performance shown in Figure 2(c) and the slightly larger RMSE in Table II.

For this SAN polymerization process, the SVM and ANN modeling yield excellent performances, whereas the PLS modeling results in the worst performance. This can be ascribed to the strong nonlinear function-



(a)



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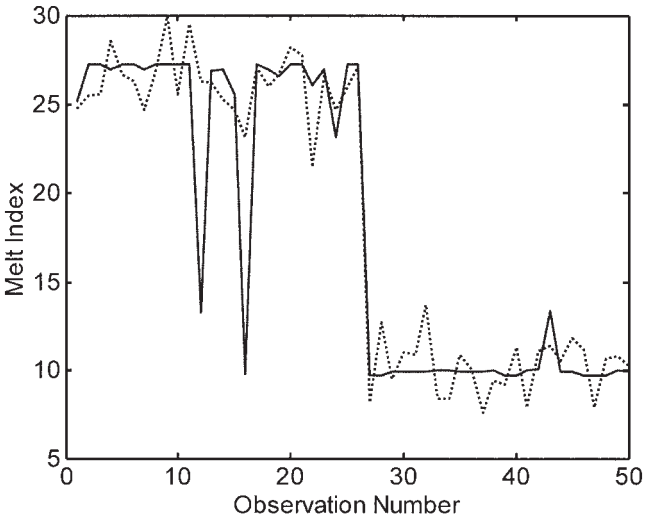

(c)

Figure 4 Results of melt index modeling (a) with the SVM method, (b) with the PLS method, and (c) with the ANN method for PP polymerization: (· · ·) measured values and (—) predicted values.

ality that the melt index has with the operating variables of the SAN process: the nonlinear SVM and ANN models can capture the nonlinearity, and the inherently linear PLS model cannot. The SVM model shows a slightly better performance than the ANN model, but the difference is not conspicuous. However, much more effort is required to obtain the final ANN model than the SVM model: the optimization problem described by eq. (12) is plagued by numerous local minima and so needs more trial runs with different initial guesses and a longer CPU time (33.8 s) per run to reach a near global minimum, as shown in Table I. On the other hand, the convex quadratic optimization problem described by eqs. (2)–(5) for the SVM model only requires a single run with a shorter CPU time (5.4 s) to locate the global minimum.[11]

PP polymerization process

Figure 3 depicts a PP polymerization process currently operated for commercial purposes in Korea. This process has a capability of manufacturing about 210,000 tons of PP per year. The process consists of four continuous reactors in series and other miscellaneous utility units. Propylene and hydrogen are fed as the reactants into each reactor, but the catalyst is added only to the first reactor along with the solvent. The polymerization reaction takes place in a liquid phase in the first two reactors and is completed in a vapor phase in the third and fourth reactors to produce the powdered polymer product. Then, after passing through the dryer and the pelletizer in sequence, the polymer powder is stored in the silos. The PP polymerization process produces products of about 40 different grades, which are altered more than 10 times per month. In addition, the process alternately uses two types of catalysts, showing different behaviors depending on the catalyst type. The product quality is managed through the control of the density and melt index of the polymer products in the process.

To prepare a set of modeling data, we retrieve the measurements of the process and quality variables from the RTDB and LIMS for the PP polymerization process. The process variables are measured every minute, and the quality variable (the melt index) is measured every 4 h. A total of 78 process variables are selected as the independent variables. Similarly to the SAN polymerization process, the moving averages of the measurements of the process variables are taken over a 4-h period before each sampling time for the

quality variable. A PCA is also applied to remove statistical outliers to get a total of 467 training data (measured for 1868 h). Then, a separate set of 50 testing data (measured for 200 h) is newly prepared for the verification and performance comparison of the models. The optimal tuning parameters with which the final SVM, PLS, and ANN models for the PP polymerization process are trained are shown in Table I.

Figure 4(a–c) and Table II show the prediction results from the SVM, PLS and ANN models, respectively, for the PP polymerization process. The results clearly show that the SVM model gives the best prediction performance of the three models. The predicted values of the melt index show quite good matches with the measured ones in Figure 4(a), and this is quantitatively supported by the smallest RMSE value (1.51) in Table II. Contrary to the SAN polymerization process, the PLS model shows a reasonable prediction performance, but it is not as good as the SVM model for the PP polymerization process, as shown in Figure 4(b) and Table II. However, the ANN model yields a very poor performance: the predictions deviate significantly from the measurements in Figure 4(c), and the RMSE value is twice as large as that of the SVM model in Table II.

Because typically a large amount of data is need for ANN modeling, the poor prediction performance of the ANN model can be explained by the insufficient data available for training the model for the PP polymerization process. The number ratio of the measurements to the input variables is only about 6 for the PP polymerization process, whereas the ratio reaches about 33 for the SAN polymerization process, for which the ANN model shows good prediction performance. Notwithstanding the scarce training data, however, the SVM model yields good prediction performance and a much shorter CPU time (1.5 s), and this suggests that it can be successfully applied to modeling a variety of polymerization processes.

CONCLUSIONS

The melt indices in the SAN and PP polymerization processes have been modeled with three black-box modeling techniques (SVMs, PLS, and ANNs.) This application of the SVMs to modeling polymerization processes is the first attempt reported in the open literature. The SVM models give the best prediction performances for both the SAN and PP polymerization processes. The ANN models fail to accurately predict the melt index when sufficient data are not available for model training in the PP polymerization process. The PLS models are not effective either when applied to the SAN polymerization process, in which the melt index has strong nonlinear functionality with the process variables. The good prediction performance that the SVM models have shown despite the insufficient data or strong process nonlinearity suggests that the SVMs can be effectively used for modeling the melt indices in other polymerization processes as well.

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